LCST Phase Behavior in Novel Ionic Liquid/Conventional Solvent Systems

Anabela J. L. Costa and Mário R. C. Soromenho
Instituto de Tecnologia Química e Biológica, Universidade Nova de Lisboa, Oeiras, Portugal

Karina Shimizu
Instituto Superior Técnico, Universidade Técnica de Lisboa, Centro de Química Estrutural, Lisboa, Portugal

José M. S. S. Esperança [C]
Instituto de Tecnologia Química e Biológica, Universidade Nova de Lisboa, Oeiras, Portugal
jmesp@itqb.unl.pt

José N. Canongia Lopes [S]
Instituto Superior Técnico, Universidade Técnica de Lisboa, Centro de Química Estrutural, Lisboa, Portugal

Luís Paulo N. Rebelo
Instituto de Tecnologia Química e Biológica, Universidade Nova de Lisboa, Oeiras, Portugal

The search for environmentally friendly ionic liquids led to the use of ionic liquids based on the cholinium cation (trimethyl-hydroxyethylammonium). Nevertheless, most of the ionic liquids based on the cholinium cation show higher melting points than those of common alkyl-imidazolium based ionic liquids. To overcome this problem, new families of ionic liquids inspired on alkyl-dimethyl-hydroxyethylammonium, with the alkyl chain length ranging from C_2 to C_8, combined with the bistrisflamide anion were tested. Liquid-liquid phase behavior data of these ionic liquids with distinct ethers has revealed an interesting and unexpected behavior: demixing occurred upon heating for particular ionic liquid/ether solutions. In the language of thermodynamics, this is called a lower critical solution temperature (LCST). The underlying entropy-driven mechanism for this behavior is generally attributed to specific solute-solvent interactions. Another important feature of the studied systems is that their critical compositions correspond to relatively low ionic liquid concentrations. The effect of the structure of both mixture components in the liquid-liquid phase behavior will be discussed and Molecular Dynamics simulation results were used to highlight the most relevant features of these systems in terms of intermolecular interactions.